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MOLECULAR DYNAMICS OF LIPID BILAYERS

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(u) Molecular Dynamics of Lipid Bilayers

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19 ABSTRACT (Continue on reverse if necessary and identify by block number)

The aim of this work is to study, by molecular dynamics simulations, the properties of model lipid bilayers. We have applied the vectorizable, order-N Monotonic Lagrangian Grid near-neighbors algorithm and have developed a novel constraint algorithm to a simple model bilayer system. We have developed fast angle-dependent force/potential algorithms to treat angle bending and torsion.

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Principal Investigator: Mark Nagumo
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Project Objectives:

The objective of this research is to study lipid bilayer models by molecular dynamics simulations. The computer code, which has been developed on the Cray XMP-24 at the Naval Research Laboratory (NRL), is based on the Monotonic Lagrangian Grid (MLG) near neighbors algorithm developed by Boris and Lambrakos of the Laboratory for Computational Physics and Fluid Dynamics at NRL [1,2]. The MLG algorithm had been developed for simulating diatomic systems such as N_2 [3]. A characteristic deeply embedded in the current realization of the MLG algorithm is two-dimensional periodicity. The direction normal to the periodic plane can be bounded by a reflecting wall or it may be free. A constraint algorithm had been developed and tested to maintain a fixed distance between the constitutive atoms of the diatomic molecules.

There were two paramount problems to solve in order to adapt the molecular dynamics codes to simulations of systems of polyatomic molecules such as lipid bilayers. First, it was necessary to generalize the constraint algorithm to the polyatomic case. This work has been described in publication #1, below. Second, it was desirable to develop an efficient method for calculating the intramolecular angle dependent functions for potentials and forces of torsion and angle bending. The angle-dependent force algorithm determines the directions along which forces are to be applied to particles by projection methods, rather than by calculating cross products. The projection code used fewer expensive operations: the angle-bending algorithm is approximately 7 times faster and the torsion algorithm approximately 40% faster than the cross-product based code. This work has been completed, and a manuscript is in preparation for submission to **Siam J. Sci. Stat. Comp.**

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A forty picosecond simulation of a butane system has been conducted to test the performance of the constraint and torsion algorithms. The Ryckaert-Bellemans torsional and intermolecular potential (Lennard-Jones with a cross section of 3.92 Å and well depth of 72 K) were used [4]. The energy of the system versus time is shown in figure 1. The initial angular distribution was chosen with a gaussian random distribution about the trans (0°) minimum of the torsional potentials, and the molecules were assigned random center of mass velocities. The total energy is reasonably well conserved; improvements are possible by using a shorter time step or by using multiple time steps to separate rapid and slow degrees of freedom. The development of the distribution of torsion angles towards the equilibrium Boltzmann distribution is shown in figure 2 at 0, 1, 5, 10, 25, and 40 ps.

Simulations of a C_{10} bilayer are underway.

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1. J.P. Boris (1986) **J. Comput. Phys. 66**, 1-20.

2. S.G. Lambrakos and J.P. Boris (1987) **J. Comput. Phys. 73**, 183-202.

3. S.G. Lambrakos, J.P. Boris, R.H. Gurguis, M. Page and E.S. Oran, (1988) **J. Chem. Phys. 90**, 4473-4481.

4. J.-P. Ryckaert and A. Bellemans (1978) **Discuss. Faraday Soc. 66**, 95-106.

Publications:

1. "A Constraint Algorithm for Maintaining Rigid Bonds in Molecular Dynamics Simulations of Large Molecules," S.G. Lambrakos, J.P. Boris, E.S. Oran, I. Chandrasekhar and M. Nagumo, NRL Memorandum Report 6174, March 4, 1988.

2. "A Modified Shake Algorithm for Maintaining Rigid Bonds in Molecular Dynamics Simulations of Large Molecules," S.G. Lambrakos, J.P. Boris, E.S. Oran, I. Chandrasekhar and M. Nagumo, **J. Comput. Phys.**, 1989, in press.*

3. "An Algorithm for Calculating Angle-Dependent Forces on Vector Computers" J.H. Dunn, M. Nagumo and S.G. Lambrakos, in preparation.*

*preprint or reprint available on request to MN

Figure 1

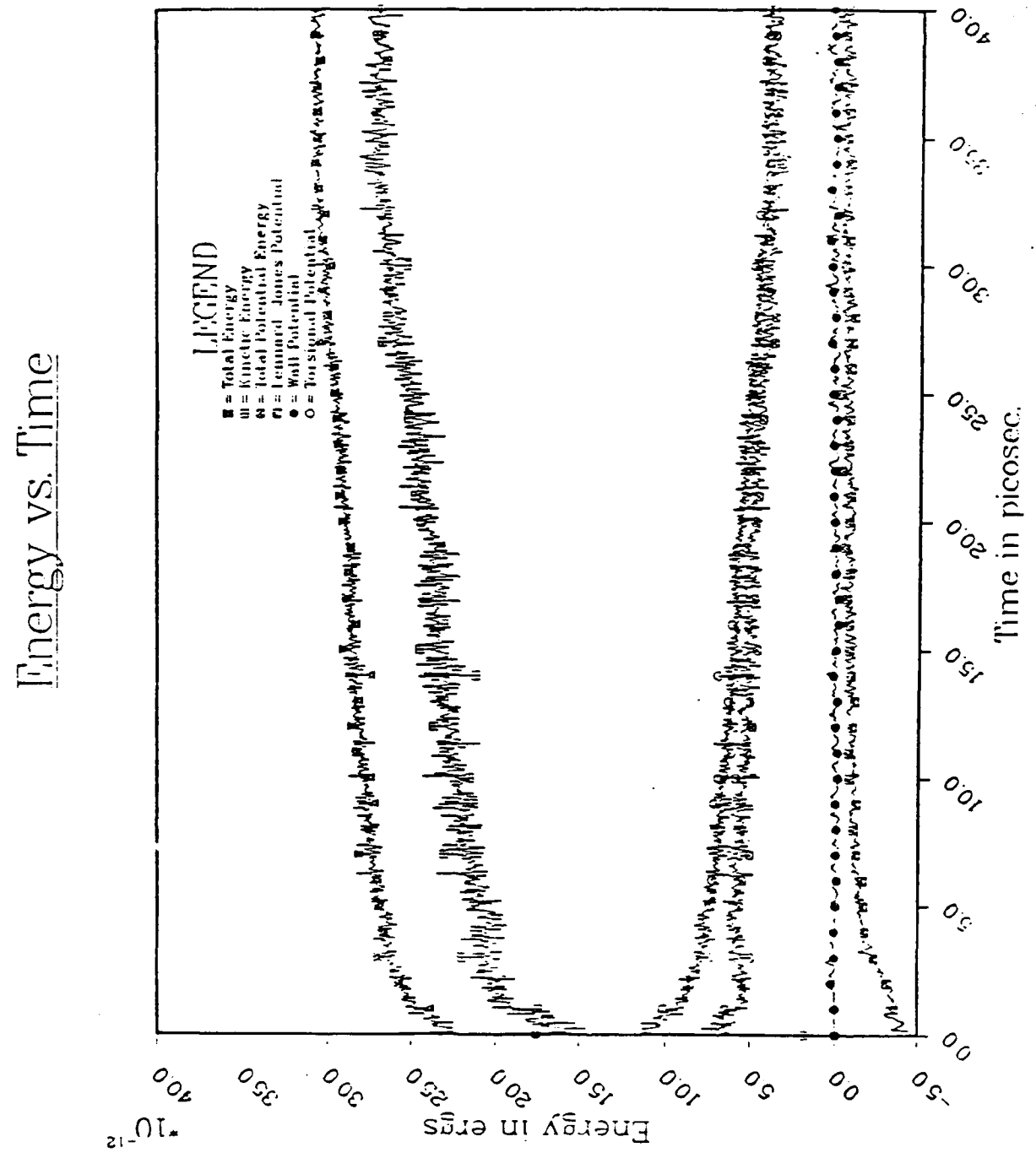
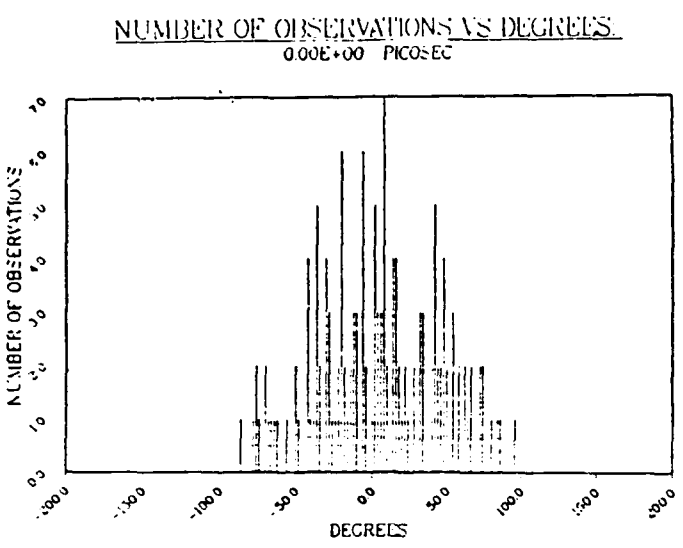

Energy vs. Time
LEGEND
■ = Total Energy
□ = Kinetic Energy
N = Total Potential Energy
□ = Lennard Jones Potential
● = Wall Potential
○ = Torsional Potential
Energy in ergs
*10^-12
-50
0.0
50
100
150
200
250
300
350
400
0.0
5.0
10.0
15.0
20.0
25.0
30.0
35.0
40.0
Time in picosec.

Figure 2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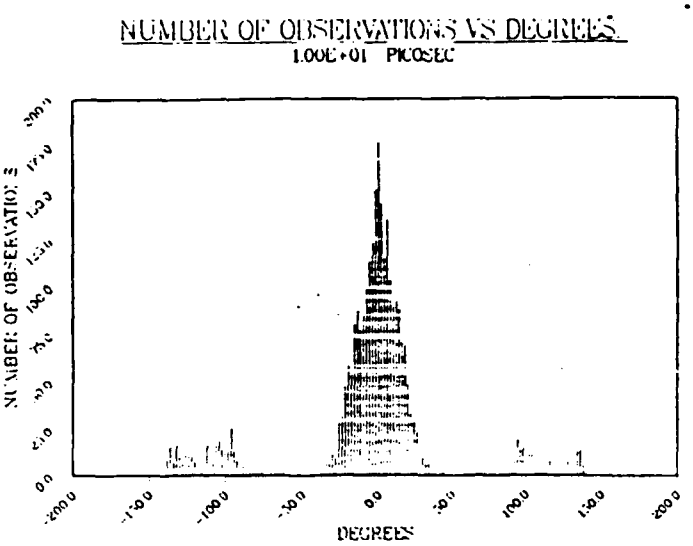
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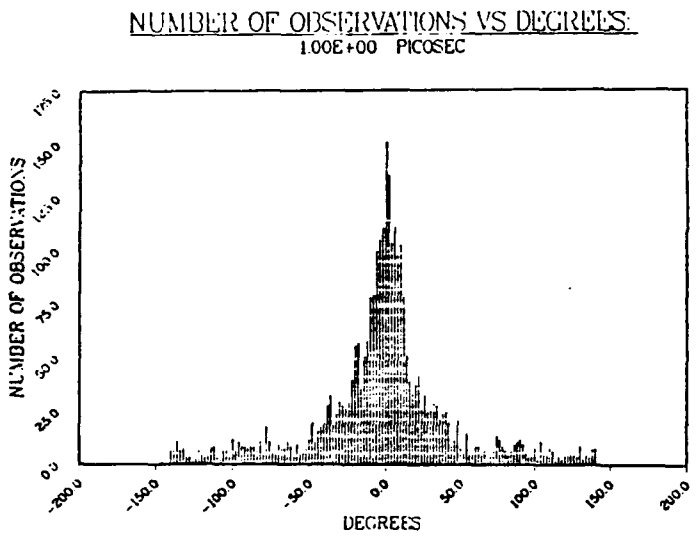
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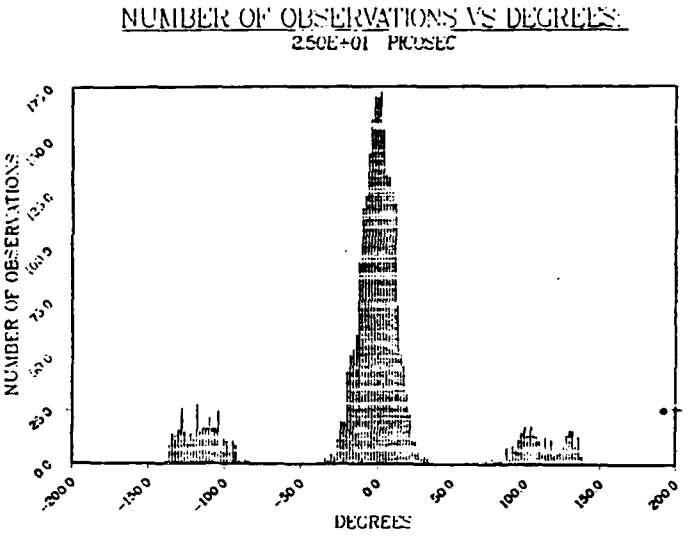
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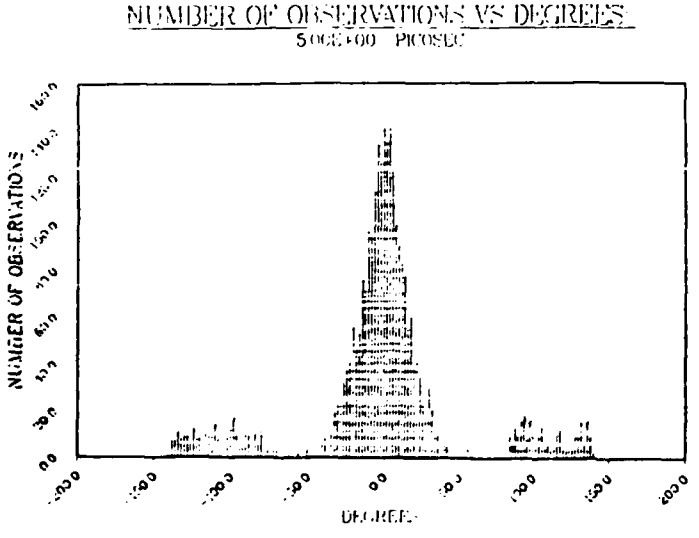
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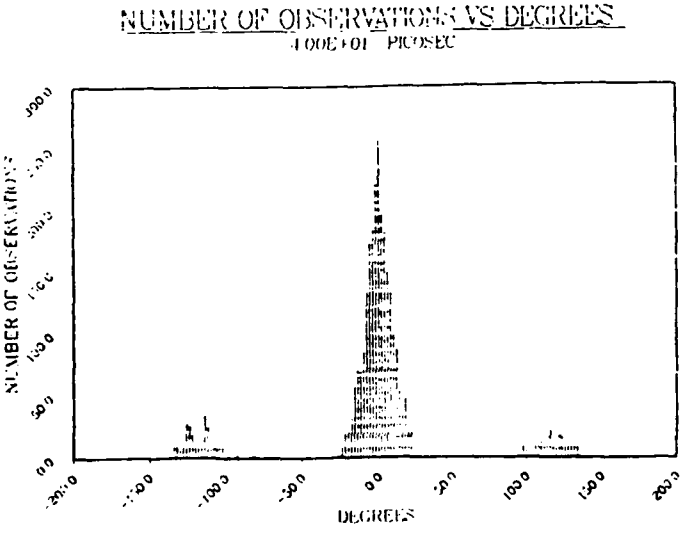
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